Reduction of Ozone Data

Procedures involved in reducing relatively clean air Dobson spectrophotometer observational data to yield total ozone amounts are straightforward. Observers are, therefore, urged to compute the total ozone amount immediately after making each observation and to examine the results for reasonableness. If the calculated ozone amount appears unrealistic, another observation following the first one should be made to improve on or verify the result first obtained. With modern computers, this is much simpler than in the past, and in many systems an ozone value is produced with directly at the end of the observation. Often the computer program has a set of criteria to apply to the observation, and can reject the observation as being too variable, or highly unreasonable. These programs then suggest possible reasons and solutions. Observers can make two observations, and easy compare the results. Results that agree with +/-1% indicate reliable observations.

The equations and coefficients described in this section have limitations. Other methods can be appropriate under special circumstances. Ozone values placed in the World Ozone and UV Data Center are expected to have been analyzed with the equations and coefficients given here, so the values can be compared with those from other stations and times. When results from other instruments are compared to the Dobson instrument results, the limitations can become evident. [*Bernard, 2004 – in progress*]

Total ozone measurements in highly polluted atmospheres may be degraded by atmospheric trace gas constituents such as SO_2 and NO_2 that have absorption spectra in the region of the Dobson instrument wavelengths, or by ozone produced photochemically near ground level in polluted air (Komhyr and Evans, 1980). Observers, whose Dobson instruments are located in highly polluted air, are encouraged to conduct investigations into the amounts of interfering trace gases present and to make estimates of possible total ozone measurement errors. Stations in polluted air have special problems. Polluted air is often not well mixed or consistent, changing with air flow and sun light. As the region producing the pollutant changes over the years, a false trend can be introduced in the data record [*De Muer, 1992*]. Some stations are subject to polluted air when local weather conditions allow. Other measurements made at the site can be used to determine if the station was under the influence of polluted air.

The analysis of the observations on direct sunlight to produce total ozone is based fully on the physics of the measurement. The analysis of the observations on zenith sky light is based on the statistics of quasi-simultaneous direct sun and zenith observations. This method forces the long-term average of the zenith observations to match that of the direct sun. This likely is a false result with regards to cloudy zenith, as the atmospheric conditions that make quasi-simultaneous possible are likely different than the conditions that produce consistent cloud. In regard to measurements on the light from the zenith, the knowledge of the radiative transfer processes has increased, but the cloudy conditions are still a problem – not only for Dobson observations, but for all instruments that look at skylight under cloudy conditions, and attempt to deduce total ozone.

The chart method described below has the statistical background buried. This technique dates from a time when complex computations were more difficult and time consuming. The relationship can be described with a set of polynomial equations, the coefficients being determined from quasi-simultaneous measurements [*Stanek and Vanicek, 1996*]. The coefficients are station dependent, and should be continuously verified, as the atmosphere changes on the long term.

The results of the analysis are dependent on the assumptions used in the analysis method. These assumptions and their effects should be considered when ozone values from other instruments are compared to Dobson results.

There are limitations to the instrument ability to correctly measure the difference of intensity, especially a low intensity light [*Basher*, 1982]. This is especially true of the A-pair. An indication of the intensity of the light is the term MuX, the mathematical product of the total ozone amount and Mu. Stations that make observations at high Mu values, should investigate the response of their instrument with respect to MuX. The CD measurements are much dependent on MuX, and can be used as a baseline.

Sometimes observations are made as single pair measurements, such as CDA (a C-pair, followed by a D-pair, and then an A-pair). Each measurement in the observation has a separate time. The equations must be derived so that the mu value for each individual pair is calculated and included in the calculation. This calculation is described in detail in the discussion of instrument calibration.

7.1 Calculations of Total Ozone from Measurements on Direct Sun or Moon

The general equations used for deducing total ozone amounts from Dobson spectrophotometer observations on direct sun or moon are given in Section 2.1 of this manual. Insertion into these equations of numerical values for the ozone absorption coefficients alpha and for the molecular scattering coefficients beta yields the following equations from which total ozone amounts are computed:

$$X_A = \frac{N_A}{1.748\ \mathrm{mu}} - 0.066\frac{m\ p}{\mathrm{mu}\ p_0} - \frac{(\mathrm{delta}-\mathrm{delta}')_A}{1.748} * \frac{\sec Z}{\mathrm{mu}} \quad (3)$$

$$X_B = \frac{N_B}{1.140\ \mathrm{mu}} - 0.099\frac{m\ p}{\mathrm{mu}\ p_0} - \frac{(\mathrm{delta}-\mathrm{delta}')_B}{1.140} * \frac{\sec Z}{\mathrm{mu}} \quad (4)$$

N_C $\quad m\ p$ $\quad (\mathrm{delta}-\mathrm{delta}')_C$ $\quad \sec Z$

```
X_C = -------- - 0.138----- - --------------- * -----
(5)
     0.800 mu        mu p_0       0.800          mu
```

$$X_D = \frac{N_D}{0.360\ mu} - 0.289\frac{m\ p}{mu\ p_0} - \frac{(delta-delta')_D}{0.360} * \frac{\sec Z}{mu} \qquad (6)$$

$$X_{AD} = \frac{N_A - N_D}{1.388\ mu} - 0.009\frac{m\ p}{mu\ p_0} - \frac{[(delta - delta')_A - (delta - delta')_D = 0]}{1.388} * \frac{\sec Z}{mu} \qquad (7)$$

$$X_{BD} = \frac{N_B - N_D}{0.780\ mu} - 0.012\frac{m\ p}{mu\ p_0} - \frac{[(delta - delta')_B - (delta - delta')_D = 0]}{0.780} * \frac{\sec Z}{mu} \qquad (8)$$

$$X_{CD} = \frac{N_C - N_D}{0.440\ mu} - 0.014\frac{m\ p}{mu\ p_0} - \frac{[(delta - delta')_C - (delta - delta')_D = 0]}{0.440} * \frac{\sec Z}{mu} \qquad (9)$$

AD-DSGQP observations have been recommended as standard by the International Ozone Commission. All other observations must therefore be reduced to the AD level before publication of final data. As indicated in Section 6.4.4, for example, CD-DSGQP observations may yield total ozone data slightly different from total ozone amounts determined from ADDSGQP observations. This difference should be determined by special measurements such as those described in Section 6.4.4, and the XCD values adjusted to the XAD level before publication of the data. Determinations of X_A, X_B, X_C, and X_D are not normally made since numerical values for the particle scattering coefficients associated with these observations are generally unavailable. Exceptions are moon observations on D wavelengths in polar regions where the air is very clean. When the moon is fairly low in the sky, there may not be sufficient instrument sensitivity to make observations using A-pair and C-pair wavelengths, but adequate response of the instrument to the longer D wavelengths. Reduction of the data then involves use of equation (6), with the assumption that $(delta-delta')_D = 0$.

7.1.1 Ozone Absorption Coefficients

IAMAP 1968 ozone absorption coefficients used in reducing Dobson spectrophotometer data are shown in Table 5. The coefficients have been derived from Vigroux (1953) laboratory values, modified for use with Dobson spectrophotometers by Dobson (1957a), and adjusted at the recommendation of the IOC in 1968 on the basis of observational data to yield relatively consistent sets of ozone amounts from observations made on different wavelengths. This section will have to be updated with the 1992 coefficients.

In calculating the ozone absorption coefficients, allowance was made by Dobson for the temperature of ozone in the atmosphere (assumed to be -44°C) and for the finite band-width of wavelengths passed by the monochromator. The equivalent widths of the monochromator slits are:

S_1 = 9 A.U. S_2 = 9 A.U. S_3 = 30 A.U.

Weighting of the absorption coefficients for the different wavelengths is that shown in Figure 6.

The absorption coefficients shown in Table 5 have been adopted as standard. Recent evidence, subject to verification, suggests that these coefficients possibly yield ozone amounts too high by 5 to 10 percent (Komhyr, 1980). The coefficients were re-determined, and new values were put into place in 1992 (http://www.cmdl.noaa.gov/ozwv/dobson/papers/coeffs.html)

7.1.2 Rayleigh Scattering Coefficients

The molecular scattering coefficients incorporated into equations (3) to (9) above are presented in Table 5.

7.1.3 Particle Scattering Coefficients

In reducing ozone data from observations on double pair wavelengths such as the AD and the CD wavelengths, the particle scattering coefficients

$(\text{delta-delta}')_A - (\text{delta-delta}')_D$
$(\text{delta-delta}')_C - (\text{delta-delta}')_D$
are assumed to be zero.

Except during very clear atmospheric conditions that may be present in polar regions, over oceans, on top of high mountains, etc., the pair wavelength coefficients $(\text{delta-delta}')_A$, $(\text{delta-delta}')_C$, and $(\text{delta-delta}')_D$ are not zero. Ozone measurements, therefore, should generally not be made using single pair wavelengths (see also Section 7.1).

7.1.4 Computation of mu

The quantity mu represents the ratio of the actual path length of a ray of light through the ozone layer as compared to the vertical path length. It is computed from the equation:

$$mu = \frac{R + h}{\sqrt{(R+h)^2 - (R+r)^2 \sin^2 Z}} \qquad (10)$$

where
R = mean earth radius (6371.229 km);
r = height of the station above mean sea level;
h = height of the ozone layer above mean sea level at the location of the station;
Z = solar zenith angle.

No significant errors are introduced into computations of mu by using the mean earth radius for R rather than the actual earth radius at the station location. It is important, however, to incorporate into equation (10) correct values for the station height above mean sea level, r, and the height of the ozone layer, h, above mean sea level at the station location. It is well known that the height of the ozone layer above mean sea level decreases in the pole-ward directions. To solve equation (10) it is sufficient to use values for h given in the table below, which relates the height of the ozone layer above mean sea level to station latitude.

Station Latitude, theta in Degrees	Height h of Ozone Layer Above Mean Sea Level in Km
± 0	26
± 10	25
± 20	24
± 30	23
± 40	22
± 50	21
± 60	20
± 70	19
± 80	18
± 90	17

7.1.5 Values of m and p/p_0

The symbol m appearing in equations (3) to (9) represents the equivalent path length of sunlight or moonlight through the earth's atmosphere allowing for refraction and curvature of the earth. Values of m vs. COSZ (Bemporad, 1907) are tabulated in Appendix G. Values of m may also be determined from the following polynomial approximation to the values of Bemporad (Hiltner and Hardie, 1962):

$$\begin{aligned} m = \sec Z &- 0.0018167(\sec Z - 1) \\ &- 0.002875(\sec Z - 1)^2 \\ &- 0.0008083(\sec Z - 1)^3 \end{aligned} \qquad (11)$$

When computing ozone amounts from observations on the double pair wavelengths AD, or CD, it is sufficient to use mean station pressure p in equations (7) to (9). However, when computing single pair A, C, or D wavelength ozone amounts using equations (3) to (6), significant errors result if mean rather than actual pressures are used at times when extreme pressure deviations occur at the station.

Deleted: B,

7.1.6 Computation of COS Z for Sun and Moon

Details of manual and computer calculations of solar and lunar zenith angles Z, and hence mu, are provided in Appendix F. The importance of incorporating horizontal parallax corrections into the COSZ computations for moon observations is also treated in this Appendix. Additional useful astronomical information, concerning the celestial sphere and concept of time, is provided in Appendix H and Appendix I.

7.2 Calculation of Ozone Amounts From Measurements on the Clear Zenith Sky

Zenith sky ozone observational data are reduced by means of empirically constructed charts which relate instrument N values, mu and X. Such charts are normally drawn up using quasi-simultaneously obtained data from AD-DSGQP observations and observations on the clear or cloudy zenith. Nearly simultaneous direct sun and clear zenith sky observations are readily obtainable. However, when the sky is cloudy, it often becomes necessary to compare direct sun and cloudy zenith observations that have been taken several hours apart.

The data reduction charts shown in the following sections were derived in Canada in the late 1950's (Komhyr, 1961; Kinisky et al., 1961), and are applicable for use in middle latitudes. Copies of the charts are available from NOAA Air Resources Laboratory, Boulder, Colorado, for preliminary use at any ozone observatory. It is important to note that the charts cannot be used universally, since the shapes of the chart curves are a function of the ozone vertical distribution, the earth's albedo, atmospheric clarity, and instrumental factors. Therefore, although the charts can serve as useful starting tools for preliminary reduction of data, it is necessary at each station to obtain a sufficient number of comparison direct sun and zenith sky observations to correct the charts so that they yield optimum quality data at that location.

7.2.1 AD-ZB Observations

AD-ZB observational data are reduced by converting instrument R-dial readings to N_A - N_D values, computing COS Z and mu from knowledge of the times of observations, determining (N_A - N_D)/mu values, and then reading total ozone amounts directly off Chart AD, a sample copy of which is shown in Figure 7.

Some indication of the quality of data obtainable from AD wavelength observations on the clear zenith sky has been given by Komhyr (1961) who showed that when 177 nearly simultaneous ADDS and ADZB values were compared at Moosonee, Canada, during 1957 to 1959, over a wide range of mu and X, the resulting error frequencies for the zenith sky observations were the following:

Error :	<= 1%	<="2%"	<="3%"
Frequency :	54%	78%	95%

7.2.2 CD-ZB Observations

These are reduced in a manner similar to that used in reducing AD-ZB observations. The ozone values are read off Chart CD, a sample copy of which is shown in Figure 8. Chart CD should, however, be regarded as highly tentative since a definitive study has not yet been made of how well total ozone amounts can be estimated from zenith sky observations on CD wavelengths.

7.2.3 CC'-ZB Observations

Here again, R_C and $R_{C'}$ readings are first converted to N_C and $N_{C'}$, mu is computed, and using the mu and $N_{C'}$ values a small, usually negative haze-correction factor, DeltaN$_C$, is read for low cloud off Cloud Correction Chart C', a sample of which is shown in Figure 9. DeltaN$_C$ is then added to the observed N_C and the new N_C value and corresponding mu are finally used in reading the ozone amount directly off Chart C, a sample of which is shown in Figure 10.

If the sky is perfectly clear, the correction DeltaN$_C$ should equal zero. In practice, even though the sky may appear to be very clear, DeltaN$_C$ is found to be small, positive or negative. The reason for the observed scatter is unknown; it cannot be attributed entirely to instrumental error. When reducing the data, positive DeltaN$_C$ values are taken to be equivalent to zero.

The abscissa values shown in the Cloud Correction Chart C' chart of Figure 9 apply to a specific ozone spectrophotometer. For another instrument, these values will normally be shifted by a constant. To determine the shift constant, it is necessary to perform many clear zenith sky observations on C' wavelengths (for 1.015 < 4.4). Fitting of the resulting $N_{C'}$ values to the DeltaN$_C$ = 0 curve of the Cloud. Correction Chart then establishes that chart's abscissa values for the particular instrument in use.

Some indication of the quality of data obtainable from CC' wavelength measurements on the clear zenith sky is available from observations made at Moosonee, Canada. When 201 ADDS and CC'ZB nearly simultaneous values were compared during 1957 to 1959 over a wide range of mu and X, the resulting error frequencies for the zenith sky observations were the following:

Error :	<= 1%	<="2%"	<="3%"
Frequency :	60%	82%	92% .

.3 Calculation of Ozone Amounts from Measurements Made on the Cloudy Zenith

7.3.1 AD-ZC Observations

The ozone data are at first reduced in exactly the same way as the clear sky observations. Measurements on cloud, however, tend to yield ozone values that are slightly too high, especially at the higher mu values. The X_{AD} values read off Chart AD must be decreased by amounts shown in a Table of Cloud Corrections for AD Observations, a sample copy of which is shown in Table 6. The cloud corrections are applied only for medium-thick or thick clouds.

An indication of the quality of data obtainable from AD wavelength measurements on the cloudy zenith sky is available from observations made at Moosonee, Canada. When 136 quasi-simultaneous ADDS and ADZC values were compared during 1957 to 1959 over a wide range of mu and X, the resulting error frequencies for the zenith sky observations were the following:

Error :	<= 1%	<="2%"	<="3%"	<="4%"
Frequency :	32%	55%	76%	91% .

7.3.2 CD-ZC Observations

The ozone data are reduced in exactly the same way as the clear sky measurements. Further work is needed to ascertain whether a table of cloud corrections (similar to that used in reducing AD-ZC data) is needed to improve the quality of CD-ZC type observations.

7.3.3 CC'-ZC Observations

The observations are reduced in a manner similar to that for reduction of CC'-ZB observational data. However, the cloud correction (deduced from Chart C') to be applied to N_C values now becomes DeltaN_C + delta(DeltaN_C) where delta(DeltaN_C) vanishes for low cloud but not for middle or high cloud.

An indication of the quality of data obtainable from CC' wavelength measurements on the cloudy zenith sky is available from observations made at Moosonee, Canada. When 300 quasi-simultaneous ADDS and CC'ZC values were compared during 1957 to 1959 over a wide range of mu and X, the resulting error frequencies for the zenith sky observations were the following:

Error :	<= 1%	<="2%"	<="3%"	<="4%"
Frequency :	33%	66%	81%	89% .

An alternate method of applying cloud corrections to CC'-ZC type observations is presented by Dobson (1957a). Application of this method, however, is somewhat more tedious than that described above, and does not lead to markedly improved data.

7.4 Reduction of Umkehr Data

In processing standard Umkehr data for C wavelengths, the N_C values of interest are those corresponding to solar zenith angles Z of 60°, 65°, 70°, 74°, 75°, 77°, 80°, 83°, 84°, 85°, 86.5°, 88°, 89°, and 90°. To extract the needed information from the entire body of observational data, the practice is to plot instrument dial readings R_C vs. Greenwich Mean Time as shown in the sample plot of Figure 11. Then, starting with values of COSZ, the times of occurrence of the pertinent Z values are computed by working the usual mu computations in reverse (See Appendix F). R_C values, corresponding to the computed times, are then extracted from the plotted data and converted to the required N_D values. Short Umkehr N_A and N_D values are obtained in a similar manner from plots of R_A and R_D vs. Greenwich Mean Time.

Observational Umkehr data should be coded according to instructions given in Section 8.2, and forwarded to the World Ozone and UV Data Center, Downsview, Ontario, Canada for processing to obtain atmospheric ozone vertical distributions processed with the most current algorithms. The code for reduction of the Umkehr measurements to profiles is available, but the actual observational data is submitted and archived, so all existing profiles can be re-determined when the algorithm is updated.

Deleted: standard Umkehr and short Umkehr

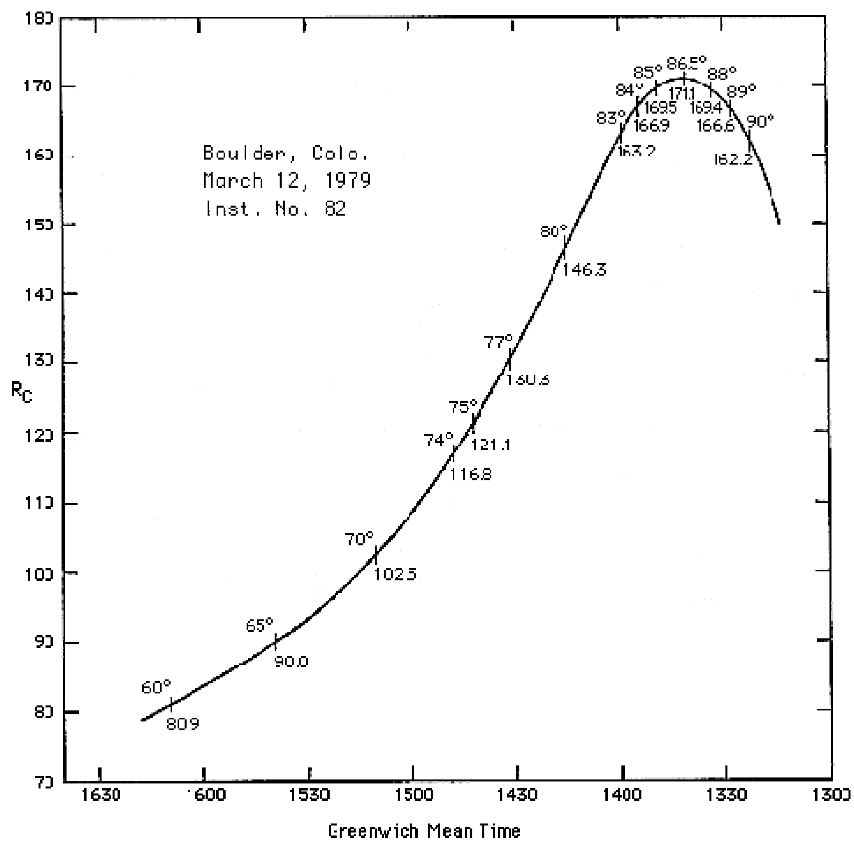

Figure 11. Sample plot of Umkehr data.